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Science & Technology REVIEW

Lawrence
Livermore
National
Laboratory

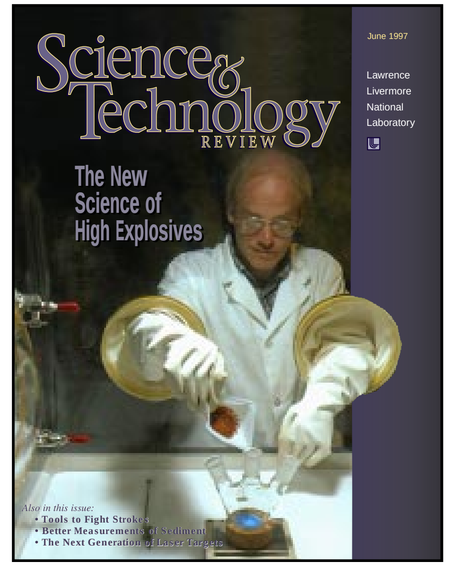
The New Science of High Explosives

Also in this issue:

- **Tools to Fight Strokes**
- **Better Measurements of Sediment**
- **The Next Generation of Laser Targets**

About the Cover

The High Explosives Application Facility (HEAF) at Lawrence Livermore is the center of some of the most advanced research in the nation and, indeed, the world.in state-of-the-art energetic materials. Since its completion in 1989, it has been the home of the development and characterization of new high explosives, a process based less on trial and error in recent years and more on rigorous scientific principles and methods. On this month's cover, Philip Pagoria, an organic chemist at HEAF, synthesizes a new high-energetic compound in a glovebox. For a report on the Laboratory's capabilities in researching energetic materials of significance to U.S. government and industry, turn to the article beginning on p. 4.



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About the Review

Lawrence Livermore National Laboratory is operated by the University of California for the Department of Energy. At Livermore, we focus science and technology on assuring our nation's security. We also apply that expertise to solve other important national problems in energy, bioscience, and the environment. *Science & Technology Review* is published ten times a year to communicate, to a broad audience, the Laboratory's scientific and technological accomplishments in fulfilling its primary missions. The publication's goal is to help readers understand these accomplishments and appreciate their value to the individual citizen, the nation, and the world.

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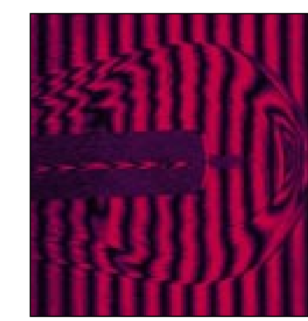

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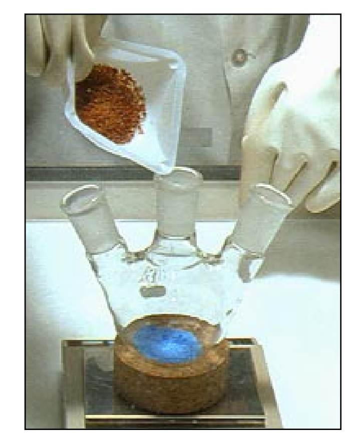

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Peña gives go-ahead for subcritical tests

Secretary of Energy Federico Peña in March gave the go-ahead for conducting subcritical experiments. Conducted nearly 1,000 feet underground, the experiments will test the basic properties of small quantities of plutonium driven to high pressures using conventional explosives. No nuclear energy will be generated by the experiments. Data on the properties of plutonium will improve the accuracy of the computer simulations that ultimately will provide a level of confidence in weapons reliability and safety, previously assured by nuclear testing.

"Subcritical experiments are essential to our commitments to a world free of nuclear testing, a reliable nuclear deterrent, and are fully consistent with the Comprehensive Test Ban Treaty (CTBT)," Peña said in a statement.

"In addition, these experiments complement other elements of DOE's Stockpile Stewardship and Management Program, such as the National Ignition Facility and the Accelerated Strategic Computing Initiative, additional tools that will help supply the confidence in stockpile safety and reliability the President has required in order to support the CTBT," he said.

The first in a series of subcritical experiments is scheduled by Los Alamos for June. The second, by LLNL, will follow sometime later.

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Scientists simulate earthquake ground-motion patterns

Scientists at Lawrence Livermore and the University of California at Berkeley have announced results of a study that models the localized severity of ground motion during a major earthquake along the Hayward fault. The fault runs beneath a densely populated section of the eastern San Francisco Bay Area.

Using one of the world's most powerful supercomputers at Lawrence Livermore, Laboratory computer scientist Shawn Larsen teamed with Berkeley seismologists Mike Antolik and Doug Dreger to simulate expected ground motions for a magnitude 7.1 earthquake along the Hayward fault beginning south of Fremont and rupturing 50 miles northwest to San Pablo Bay.

The researchers developed a computer movie based on this scenario that shows seismic waves propagating throughout the Bay Area and impacting different regions with varying degrees of severity.

"Ultimately it's our goal that those responsible for earthquake retrofit and new structure design can take our findings and combine them with current approaches to make better engineering decisions," said Larsen.

The researchers announced their findings at the Seismological Society of America annual meeting, held in April in Honolulu. Their simulations use a sophisticated computer code developed at Livermore and a seismic velocity model developed at Berkeley.

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Defense research yields commercial benefits

Defense research at Lawrence Livermore may help U.S. companies get a head start in the fiercely competitive international computer chip market, according to Dena Belzer, author of a new study about the Laboratory's effect on the economy.

Belzer, a principal consultant with Bay Area Economics in Berkeley, quoted industry giants Intel Corp. and Microsoft as saying that breakthroughs at Lawrence Livermore have been critical to putting more information onto tiny microchips. The companies said the Lab's cutting-edge research tools and wide pool of scientists from diverse disciplines enabled microchip breakthroughs such as EUV lithography, a technique for putting information on chips more precisely with strokes that are about a thousandth of the width of a human hair.

Belzer's report said that the planned National Ignition Facility laser could push the state of the art in several technology areas over the next 10 to 15 years but cautioned that "economic benefits can only be realized if the national labs continue to have strong interactive relationships with private industry."

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Lawrence Livermore's high profile in arms control

In an address to Lawrence Livermore employees in April, Ambassador Thomas Graham, Jr., U.S. negotiator and special representative of the President at the U.S. Arms Control and Disarmament Agency, applauded the Laboratory's contributions and its high-profile role in achieving a global treaty to end nuclear testing.

According to Graham, Lawrence Livermore was the only one of the nation's three nuclear weapons laboratories represented directly on the U.S. negotiating team for the test ban.

The Laboratory's representative, physicist William Dunlop, "was one of the top 10 people on our negotiating delegation," Graham said. "He and the Lab . . . made a very important contribution to developing negotiating positions and ultimately to the negotiations of the [Comprehensive Test Ban Treaty].

"More and more people in recent years have looked to the [national] labs for support in arms control and nonproliferation because they have a lot to offer. And a lot of it is world-class and unique," he said. He went on to name specialized sensors and other technology for monitoring treaty compliance as examples.

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The Critical Roles of Energetic Materials Science

LAWRENCE Livermore's involvement in energetic materials began at its inception in 1952, when the Laboratory instituted a research and development program in high explosives for nuclear warheads under design. Today, Livermore's high-explosives capabilities, with extensive facilities at the main site, Site 300, and recently, at the Nevada Test Site, are the equal of any institution's in the world.

What makes Livermore's energetic materials work internationally distinct is its breadth and depth. At one extreme, as described in the article beginning on p. 4, chemists and physicists are working to increase the safety and performance of energetic materials at the molecular level. At the other extreme, Livermore experts are supporting the safe dismantlement of nuclear weapons and the disposition of their energetic materials.

Stockpile Stewardship

The Department of Energy's Stockpile Stewardship and Management Program is the centerpiece of Livermore's national security mission. Underlying all of our stockpile stewardship activities is a dedication to assuring that nuclear weapons will continue to be as safe and reliable as they are today. The relationship of energetic materials to the well-being of the nation's nuclear stockpile is particularly strong. Activities range from assisting DOE plants in fulfilling their manufacturing mission to understanding the aging of high explosives in the stockpile and predicting their useful lifetime.

Current energetic materials research and development in support of stockpile stewardship focuses on several areas. In the important area of enhanced surveillance, we are developing new, minimally invasive methods of detecting the products of high-explosives decomposition as well as pursuing theoretical and experimental work to predict and characterize potential decomposition pathways. Our continuing emphasis on safety, performance, and reliability drives an intense effort to improve our ability to model the behavior of energetic materials under both normal and abnormal conditions. This research necessitates the acquisition of additional equation-of-state data and better modeling of the very complex coupling of thermodynamic, chemical-kinetic, and hydrodynamic behavior in a burning high explosive.

We also have a continuing responsibility to assist DOE's Pantex Plant in meeting the needs of the stockpile; we must also meet the requirements of our own hydrotesting programs. For example, we are currently doing research focused on improving the chemical synthesis processes for high explosives (e.g., a new route to the synthesis of the insensitive high explosive TATB), and we maintain a viable synthesis, processing, and assembly area at Site 300.

Department of Defense and Other Activities

Livermore's role in energetic materials has broadened beyond its primary nuclear weapon-related mission. Today, there are extensive activities in advanced conventional weapons, rocket and gun propellants, antiterrorist work, demilitarization, and industrial applications of energetic materials. We are actively assisting the Department of Defense in a wide range of activities in this area, particularly those focused on insensitive high explosives, environmentally sound demilitarization of surplus high explosives and propellants, and modeling the performance and safety of high explosives and propellants. Two current examples of Department of Defense projects are the development of molten salt as an environmentally benign means of destroying energetic materials and the exploration of new synthesis routes to reduce the cost of high explosives.

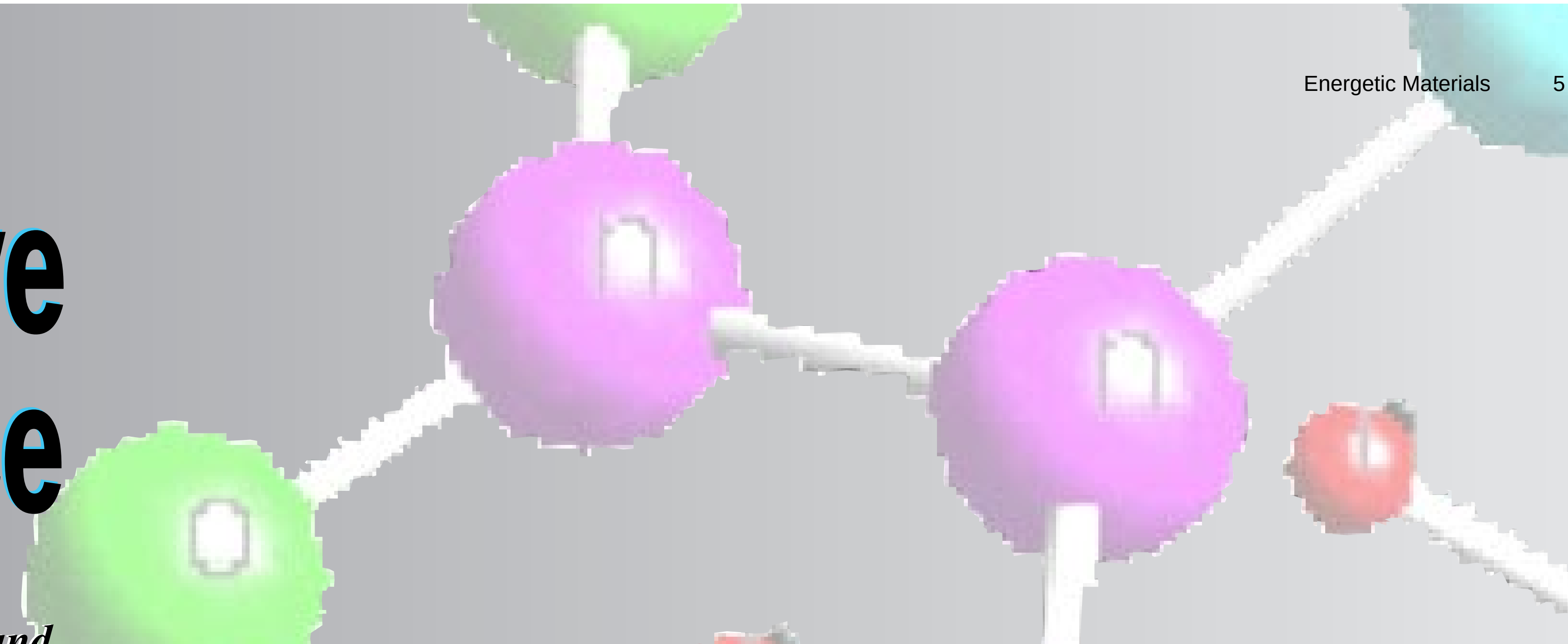
In support of Livermore's nonproliferation program, we are developing the means to reliably detect and identify high-explosive compounds and formulations, with the added interest of potentially determining their origin.

Providing the Scientific Foundation

The excellent science carried out at Livermore enables the outstanding advances in energetic materials research and development described above and in the following article. This work ranges from understanding detonation science at the molecular level to predicting structures for exciting new high explosives. This continuing excellence in the science and technology of energetic materials has made possible the wide range of Livermore contributions since its inception and promises significant breakthroughs in the years ahead.

■ Hal Graboske is Associate Director of Chemistry and Materials Science.

Transforming Explosive Art into Science



For centuries, intuition and trial and error dominated the development of high explosives. Now, high-explosives researchers at Lawrence Livermore are imposing more rigorous scientific structure and techniques upon their work.

FEW products typically take years of effort to synthesize yet disintegrate in a few millionths of a second when used. Despite their brief lifespan, energetic materials, particularly high explosives, are in demand as never before by the Department of Energy, Department of Defense, and industry for their unique properties: shock waves producing pressure up to 500,000 times that of Earth's atmosphere, detonation waves traveling at 10 kilometers per second, temperatures soaring to 5,500 kelvin, and power approaching 20 billion watts per square centimeter.

Explosives have been around since Chinese gunpowders appeared during the 11th century. However, until the past 15 years, their development has been characterized by an approach based largely on intuition and trial and error. Now high-explosives scientists are imposing more rigorous scientific structure and techniques upon all aspects of their work.

For example, Lawrence Livermore researchers are combining breakthrough computer simulation codes, state-of-the-art experimental diagnostics, and a culture in which theoretical, synthesis, and experimental chemists and physicists work alongside each other. At the same time, they are working more closely with their partners in the energetic materials community, from DOE's Pantex Plant in Texas to the Air Force's Wright Laboratory at Eglin Air Force Base, Florida, to small explosives companies in the San Francisco Bay Area.

Advances in energetic materials, which include high explosives, propellants, and pyrotechnics, benefit DOE's Office of Defense Programs, DoD's warheads and propulsion efforts (especially the 12-year-old DOE/DoD "Memorandum of Understanding on Conventional Munitions"), NASA's space exploration programs, the Federal Aviation Agency's explosive detection efforts, and many industries, including mining, oil exploration, and automobile. The continuing demand is driving a search for better theoretical models of the behavior of energetic materials and an improved diagnostic capability to measure the complex chemical and hydrodynamic processes during detonation.

According to Ron Atkins, director of the Energetic Materials Center (EMC), a joint effort of Lawrence Livermore and Sandia National Laboratories, U.S. industry has scaled back its energetic materials research because of safety and financial considerations. Likewise, the Department of Defense's own energetic materials research faces significant budget pressures, while academia does not have the costly facilities to carry out such research. As a result, says Atkins, "the national labs are becoming the country's most important repository of energetic materials expertise." Atkins is heading a task force representing several Livermore directorates in work to ensure that the Laboratory will remain a national resource for energetic materials expertise over the next decade and beyond.

Livermore researchers have studied and synthesized high explosives for decades because they are an integral element of every nuclear weapon. Today, under the EMC umbrella, their work encompasses a wide range of basic research and programmatic activities. Lawrence Livermore chemists are synthesizing new compounds that yield more energy, are safer to store and handle, and are less expensive and more environmentally friendly to produce. They also are designing new paths to synthesizing existing energetic molecules that are cheaper and easier on the environment.

Understanding Is Key Goal

Livermore scientists are conducting experiments to better understand the fundamental physics and chemistry of energetic materials, particularly with regard to their stability, sensitivity, and performance. "Despite a century of work, scientists still do not understand what happens in a detonation wave thoroughly enough to predict all the details of how a given explosive will behave under various conditions," says Randy Simpson, head of the Energetic Materials Section in the Chemistry and Materials Science Directorate.

Simpson and his colleagues are also involved in fundamental surveillance activities associated with the maintenance of the nation's nuclear weapons stockpile. Performance and safety testing (see *Science & Technology Review*, December 1996, pp. 12–17) assures that the high explosives in nuclear warheads will remain dependable despite decades of storage. Another aspect of stockpile stewardship work is developing safe and environmentally sound methods for dismantling and disposing of thousands of kilograms of high explosives removed from retired nuclear weapons. Going a step further, Livermore chemists are investigating processes that would permit the reuse of these high-quality, expensive materials in the commercial marketplace.

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Table 1. Codes used in developing energetic materials.

Code	Function
ALE3D	Hydrodynamic code used in safety analyses such as "cookoff" simulations spanning a remarkably wide time span. (Developed at LLNL.)
CHEETAH	Transforms predicted formation energy and density of molecules into performance measures such as detonation velocity, pressure, energy, impulse, and impetus. (Developed at LLNL.)
GAUSSIAN	Determines the three-dimensional shape of the molecule and the energy binding its atoms.
MOLPAK	Packs molecules together into a low-energy configuration.
TOPAZCHEM, PALM	Predict changes in thermal and chemical properties caused by different accident, battlefield, and aging scenarios. (Developed at LLNL.)

Figure 1. (above) Livermore's High Explosives Applications Facility (HEAF), completed in 1989, is playing a major role in developing and characterizing high explosives. (right) Specially designed containment vessels are used to safely detonate high explosives in quantities as large as 10 kilograms of TNT-equivalent.

Guiding all of these activities are computer codes that mimic energetic materials and the very rapid physical and chemical processes that govern their detonation (Table 1). The codes reflect longstanding Livermore expertise in simulating extremely short-lived events such as nuclear detonations. Continually refined by experimental data, the codes are paving the way for an unprecedented understanding of energetic materials at the molecular level.

The work is headquartered in the High Explosives Applications Facility (HEAF) at Livermore, which represents the state of the art in high-explosives research with regard to both technical capability and safety (Figure 1). Work at HEAF is complemented by activities some 15 miles away at Site 300, where large-scale high-explosives processing and testing are carried out.

Searching for New Materials

Simpson notes that in a world accustomed to daily announcements of important scientific advances, breakthrough high-energetic materials have been few despite steady progress in explosive power and insensitivity over the past century. The last energetic material to "hit it big" was HMX (cyclo-tetramethylene-tetranitramine), discovered during World War II as a contaminant in a batch of another explosive material. Since then, Simpson says, there have been TATB (triamino-trinitrobenzene, a highly insensitive high explosive for nuclear weapons) during the 1970s and a few specialty materials, but certainly nothing used as widely as TNT (trinitrotoluene) (Table 2).

The reason for the paucity of new energetic materials is the fact that they must meet so many different requirements such as high energy density, insensitivity to mechanical insults, resistance to chemical decomposition, inexpensive synthesis from readily available reagents, and the ability to be formulated with other materials for fabrication into practical devices.

Despite the difficult requirements, Livermore chemists are optimistic that they can improve the safety and performance of current and future weapons systems. It is a balancing act because the compounds must be powerful enough to do the job and at the same time insensitive enough to prevent accidental explosion. For some applications, the priority is on improving safety, especially with nuclear weapons and with explosives stored on ships.

For other applications, higher power and energy are of greatest interest. (Energy is the capacity of an explosive to do work, whereas power is the rate of energy release, or how rapidly the explosive can accelerate metal. Energy is measured in joules, power in joules per second.) In this area, several new Livermore explosives have been developed for Air Force weapons directed at penetrating "hard targets" such as underground reinforced concrete bunkers. In the same performance arena, smaller shaped charges using Livermore formulations are demonstrating velocities up to 10 kilometers per second to penetrate thick steel armor plate some 6 to 8 times the diameter of the shaped charge.

Developing new energetic materials is a complicated process in which many candidate molecules are considered, a few synthesized, even fewer formulated, and only a small handful adopted by the military or industry. The laborious process involves computer modeling, plenty of laboratory work, and thorough testing.

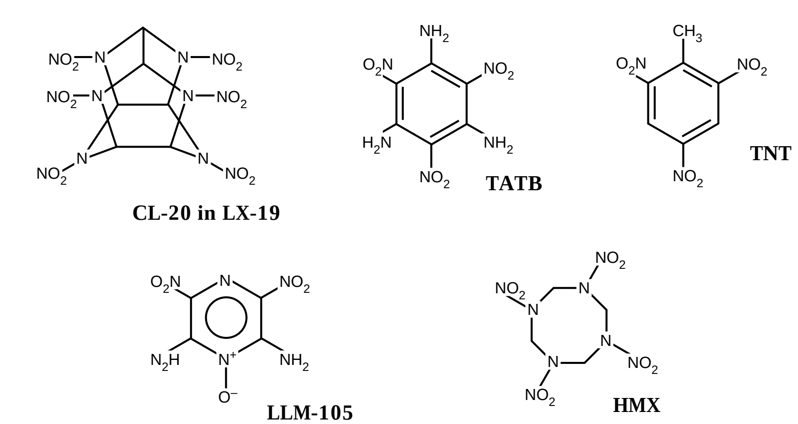
Starting at the Chalkboard

The road to a new high explosive begins the old-fashioned way, when candidate molecules are drawn on a chalkboard by both theoretical and synthesis chemists. Theoretical chemists tend to suggest more "flamboyant" molecules than the synthesis chemists because they have less experience in the laboratory, quips theoretical chemist Larry Fried. Once a group of candidates is agreed upon, Fried and his colleagues take over, screening the molecules with a host of computer codes.

The codes help guide the synthesis chemists by predicting the inherent characteristics of the cyber-compounds. Fried says the process is similar to that found in the pharmaceutical industry. In that business, too, trial and error and human hunches used to be predominant, but now sophisticated computers are helping to point the way to prime-candidate molecules for synthesis.

Livermore high-end workstations do simulations with the speed that approaches a supercomputer's. The software program GAUSSIAN (used widely in the chemical and pharmaceutical industries) is first

Table 2. Molecular structure of important energetic materials.

Material	Molecular Structures
TNT (trinitrotoluene)	
HMX (cyclo-tetramethylene-tetranitramine),	
TATB (triamino-trinitrobenzene)	
LX-19 (2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-hexaazaisowurtzitane, which is CL-20, plus a polymer binder)	
LLM-105 (2,6-diamino-3,5-dinitropyrazine-1-oxide)	

employed to determine the three-dimensional shape of the molecule and the energy binding its atoms. The molecules are then "packed together" into a low-energy configuration for greatest stability by another widely used program called MOLPAK.

Finally, CHEETAH transforms the molecules' predicted thermodynamic energy and density into explosive performance measures such as detonation velocity, pressure, and energy (Figure 2). CHEETAH, developed by Fried and his colleagues, is a thermochemistry code derived from more than 40 years of experiments on high explosives at Livermore. With libraries of hundreds of reactants and 6,000 products in its code, the program is now used throughout the world and has become DOD's preferred code for designing new explosives and, to a lesser extent, propellants and pyrotechnics (see *Science & Technology Review*, June 1996, pp. 6–13). The capabilities of the massively parallel computers in DOE's Accelerated Strategic Computing Initiative (ASCI) at the Laboratory are being used to assist with modeling the hydrodynamics of candidate explosives, and plans call for ASCI's use in creating advanced predictive models of the chemical reactions that occur when candidate molecules explode.

Assuming the software programs validate the chemists' premise that the candidate molecule offers significant potential, the material is ready to be synthesized.

Synthesis Can Be Tough

While it takes about one week to screen a candidate molecule by computer, its actual synthesis in the laboratory can require a year or even longer of painstaking effort.

"It takes a lot of trial and error to get the synthesis reactions to go," says organic chemist Phil Pagoria (Figure 3). "The chemist must constantly evaluate whether the project is progressing or whether the molecule, as planned, is impossible. It is an iterative process, depending largely on the knowledge, abilities, and intuition of the chemist. Many times, a synthesis scheme cannot be considered for full-scale production because it ultimately requires too many steps or reagents that are too costly."

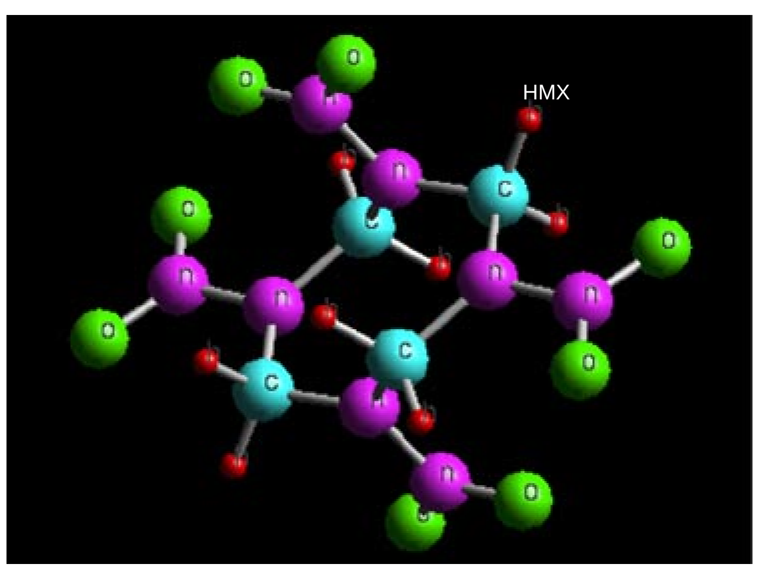
Much of the synthesis effort is devoted to developing new energetic materials that possess an energy density (the energy that can be released from a specified volume of material) at least 15% greater than that of HMX, the high-energy high explosive against which candidate materials have long been evaluated. HMX replacements are needed for a host of volume-fixed armaments such as so-called smart, or precision-guided, munitions.

Many have been developed at Livermore. One formulation, LX-19, is the highest power material in the world but somewhat more sensitive than HMX-based materials.* LX-19 is based on CL-20 (developed at the Naval Weapons Center, China Lake, California). Working with the Navy, Livermore experts determined many of the characteristics of CL-20 and performed the first scale-up to kilogram quantities at the Laboratory's Site 300 test area.

A similar effort is aimed at synthesizing materials with more energy than TNT, the best known high explosive in the world and one that offers less power (but better sensitivity) than HMX. For this effort, Livermore has synthesized LLM-105, an insensitive energetic material with 60% more energy than TNT. The new material is under evaluation by Ron Lee and his colleagues in Livermore's Defense and Nuclear Technologies Directorate.

In the process of developing new compounds and more efficient pathways for synthesizing existing compounds, the synthesis group has developed an innovative and cost-effective approach called the VNS (vicarious nucleophilic substitution) method for producing TATB. The procedure eliminates the need for chlorinated compounds, which have adverse environmental effects. (See the November 1996 *Science & Technology Review*, pp. 21–23.) Livermore and DOE's Pantex Plant recently began a four-year effort to apply the VNS method in order to establish a lower-cost industrial supply of TATB.

Once a few grams of a material have been synthesized, they are passed on to experimental chemists for a battery of safety tests (Figures 4 and 5). The tests determine the material's sensitivity to



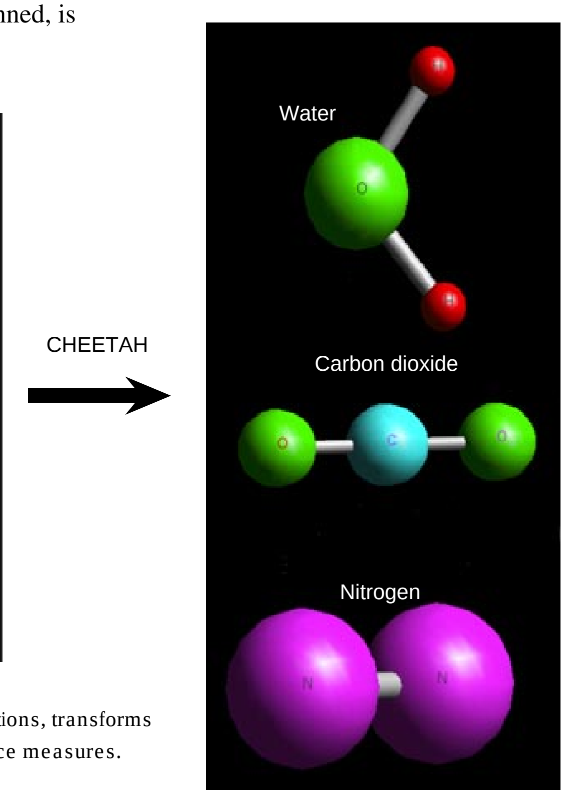


Figure 2. Livermore's computer code CHEETAH, running on high-end workstations, transforms the predicted crystal energy and density of molecules into explosive performance measures. Here the explosive molecule HMX is transformed to its detonation products.

Figure 3. Organic chemist Phil Pagoria synthesizes a new high-energetic compound inside a glovebox to guard against unwanted moisture.

Figure 4. Scientific Associate Chet Lee measures the burn rate of a high explosive under high pressure, a standard safety test.

Figure 5. Chemist Rosalind Swansiger remotely controls a performance test of a promising high explosive.

* Experimental molecules are designated by an LLM number for Lawrence Livermore molecule. Experimental formulations are designated by an RX number for research explosive. Once the material is in production, it acquires an LX designation for Livermore explosive. DoD experimental munitions receive an XM number.

impact, heat, friction, electrostatic discharge, and shock. Most candidate materials fail at this point. Those that pass are sent on to other chemists for incorporation in a mixture of ingredients called a formulation. Simpson acknowledges that the process is “still largely an art” but adds that it is becoming “more precisely scientific all the time.”

A World of Tradeoffs

Formulating high explosives for unique applications may require a medley of ingredients, including energetic crystalline powders, energetic liquids, inorganic oxides, metals, and binders such as thermoplastics, thermosets, and gels. The binder, which takes up as little as 2% and as much as 40% of the volume, can serve several purposes: it can make the explosive easier to fabricate into useful shapes, aid in desensitization to shock, or modify the high explosive’s performance characteristics.

Formulations chemist Mark Hoffman acknowledges the role of artistry in arriving at a sound formulation but notes that Livermore people can tap 45 years’ worth of experience with high explosives. Much of the artistry is spent juggling the tradeoffs among sensitivity, performance, and cost. As a formulation increases insensitivity to explosion (for safety considerations, for example), performance typically suffers. Hoffman notes: “It does no good to have a weapon on board a tank that does not possess enough power to destroy or incapacitate an opposing tank. But it’s inappropriate to carry a weapon that’s so sensitive that it explodes in response to a few bumps in the road.”

Formulators work closely with other chemists, who can quickly obtain safety and performance measurements using different quantities of a formulation. With as little as 1 to 2 grams, chemists can only perform critical safety tests. With 50-gram quantities, they can evaluate how well the ingredients of a formulation come together to form the new explosive. As formulations are scaled up to kilogram quantities, important tests of performance, thermal

stability, and mechanical and physical properties assist designers in evaluating a formulation and determining appropriate use in specific devices. Chemical reactivity tests, for example, identify incompatibilities between device components and a formulation. Because a major objective in formulation is incorporation of the formulated explosive into a device, any possible incompatibility between device components and the formulation must be corrected early.

Atkins notes that obtaining accurate data from experiments at the extreme temperature, pressure, and time regimes of high explosives presents enormous challenges. Many of the tests use diagnostic tools originally developed for underground nuclear weapons tests at the Nevada Test Site. Others were developed more recently. One such tool is the multibeam Fabry–Perot velocimeter, designed by Livermore scientists (July 1996 *Science & Technology Review*, pp. 12–19). This device provides high-resolution, continuous velocity data about the behavior of materials traveling up to 3,000 meters per second. With the multibeam system now producing more meaningful data about the power of explosives—the rate at which they are capable of releasing energy—modeling codes become increasingly accurate. The device also allows more efficient use of budgeted funds because one experiment provides many sets of velocity data, thus taking the place of five separate experiments.

Computer simulations have also strengthened formulation activity and testing. CHEETAH is once again called into play, this time to suggest how the various formulation ingredients will affect performance. In addition, TOPAZCHEM-2D/3D, PALM, and more recently, the ALE3D code (see box, below) augment safety testing by predicting changes in thermal and chemical properties caused by different accident, battlefield, and aging scenarios.

Encouraging results from experiments and computer simulations lead to still

Spotlight on Safety

The very destructive power of high explosives places a premium on all aspects of their safety, including manufacture, transportation, storage, and handling. Likewise, much of Lawrence Livermore’s high-explosives work involves determining the sensitivity of existing high explosives and rocket propellants to fire, accident, and terrorist attack.

Safety has also come under the purview of computer codes. “We would like to do predictions of safety at the start of the development process, much as we determine other characteristics of candidate molecules,” says theoretical chemist Larry Fried, who is exploring using the widespread computer code GAUSSIAN to determine how much energy it takes to break a molecular bond as an indicator of sensitivity to accidental detonation. He is also exploring the conversion of intermolecular phonons (quanta of vibration energy) to intramolecular vibrational states as part of a computational model that could eliminate inherently unstable molecules from consideration before they are synthesized.

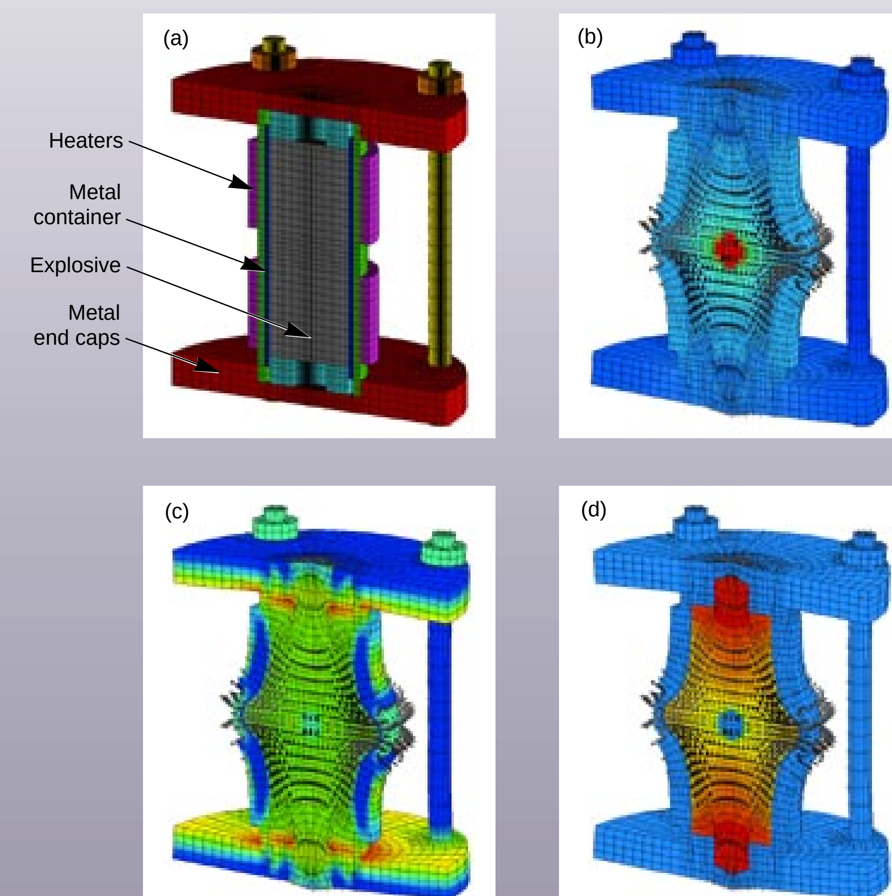
Fellow theoretical chemist Al Nichols has been working with computational scientists from the Defense and Nuclear Technologies Directorate to transform ALE3D, a three-dimensional hydrodynamic, explosive-safety code developed at Livermore (see figure on p. 11). With the ALE3D team, Nichols has added thermal and chemical capabilities to the code so it can answer safety questions about high explosives, in particular a stringent military thermal safety test called “cookoff.” Thanks to ALE3D, Livermore is the first research center to simulate cookoff by depicting a remarkably wide time span. The code models deformations in a heated explosive device from the time they begin at the rate of millimeters per day to the instant of explosion when deformation rates increase to kilometers per second.

Safety efforts include working with the Air Force on its missile propellants. One study, a part of the Titan IV program, is looking at the safety ramifications of solid propellant falling from an errant rocket launch, as happened earlier this year when an Air Force Delta rocket blew up at Cape Canaveral, Florida, raining propellant down on the ground below. Another study concerns the propellants of the Air Force Minuteman III missile.

In performing the safety studies, says experimental chemical engineer Jon Maienschein, Livermore chemists are doing business differently by modeling every experiment before it is conducted. In that respect, says Energetic Materials Section leader Randy Simpson, Livermore scientists do a smaller number of experiments than are done at other sites, but they thoroughly instrument each one and precede major experiments with computer simulations.

Maienschein notes that Livermore personnel are working more closely with colleagues and sponsors in DoD. “Both they and we recognize that we can do more by teaming up with each other.” The process, he says, encourages creative thinking about, for example, a new generation of transducer-based systems that continuously monitor important safety data such as temperature in high explosives.

Energetic Materials Center Director Ron Atkins notes that in a world of diminished federal outlays, collaboration is clearly the way to achieve important advances with the greatest cost-efficiency. “We’re working hard to build bridges to the armed services, DOE centers like the Pantex Plant in Texas, and other national labs,” he says.



The ALE3D computer code is capable of simulating a “cookoff” safety test by modeling the rate of deformations in a slowly heated high explosive over a wide time span. (a) A model of the test at setup. The high explosive is encased in steel and aluminum and bolted between two metal end caps. Heaters surround the metal container and heat the 7.6-centimeter-tall device at the rate of 3.3°C per hour. (b), (c), and (d) are snapshots of the simulation of the material’s deformation as a function of (respectively) temperature, pressure, and chemical change after 50 hours of heating. ALE3D simulations such as this tell energetic-materials scientists in great detail and in slow motion how, when, and with what violence new high-explosive compounds deform when burned. In (b), (c), and (d), the velocity of deformation is 80 meters per second.

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larger-scale formulations of 400 grams or greater done at Site 300. When the material properties are optimized, the formulation process is developed for scale-up to production quantities for final technology transfer.

Livermore chemists are also working to improve efficiencies in the production world. They are exploring the use of injection molding equipment much like that used to make plastic toy parts. Such machines could be ideal for making shaped charges, which typically contain a number of complex folds that are difficult to fashion using standard production machinery (Figure 6).

Leaving the Iron Age

Simpson describes the Iron Age as a time when builders were limited to a few metals for construction. Now builders have a host of different materials from which to choose. “We’re leaving the Iron Age of energetic materials because military planners are no longer limited to TNT and HMX,” he says. “We’re seeing specific new materials for specific military applications.”

The driving force is the ascendancy of smart munitions. Because these weapons routinely hit their targets, small improvements in the lethality of the warheads can significantly increase their effectiveness. What’s more, fewer and smaller munitions mean that more expensive energetic materials may be used.

As part of this new effort, Livermore chemists are working with the Navy to adapt LX-19 and similar CL-20 formulations to the military’s XM-80 program. Multiple small submunitions, each containing about 10 grams of explosives, will be grouped in shells and shot out of Navy guns. Capable of traveling long distances, the shells, which have a propulsion system guided by global positioning satellites, will accurately destroy enemy fortifications.

Simpson is confident that computer codes will continue to become more sophisticated so that a code such as ALE3D will be used as a design tool to model safety elements of energetic devices as diverse as rockets or automobile air bags. It is a safe bet that with other aspects of high explosives, as well, Livermore researchers will play a large part in the new age of high explosives.

—Arnie Heller

(a) (b) (c) (d)

Figure 6. At Site 300 facilities, injection-moldable explosives are developed as part of an effort to enhance production methods. (a) Mark Hoffman formulates a moldable high explosive. (b) Hoffman and Kirk Pederson pour the explosive to a transfer funnel, from which it is poured into a deaerator–loader. (c) Frank Garcia operates the deaerator–loader to remove air from the explosive before loading it into the explosive device. (d) Mike Kumpf displays the finished precision explosive device.

Key Words: ALE3D, CHEETAH, Fabry–Perot velocimeter, GAUSSIAN, high explosives, High Explosives Applications Facility (HEAF), HMX (cyclo-tetramethylene-tetranitramine), MOLPAK, PALM, stockpile stewardship, TATB (triamino-trinitrobenzene), TNT (trinitrotoluene), TOPAZCHEM.

For further information contact Randall Simpson (510) 423-0379 (simpson5@llnl.gov).

About the Scientists

The research, development, and testing of new energetic materials done at the Laboratory’s High Explosives Applications Facility is, like all science done at Livermore, a multidisciplinary team effort. In this instance, the team members operate under the auspices of the Energetic Materials Center (EMC), sponsored jointly by Lawrence Livermore and Sandia national laboratories. Chief contributors to the new science of high explosives being done at Livermore are (left to right): ALBERT NICHOLS, a theoretical chemist currently working to model safety aspects of high explosives used in nuclear and defense applications; RANDALL SIMPSON, an experimental chemist who develops new energetic materials and characterizes their initiation and detonation properties; RONALD ATKINS, director of the EMC and coordinator of the team’s work; RONALD LEE, a physicist who develops new explosive initiation systems; JON MAIENSCHEIN, an experimental chemical engineer involved in computer simulations of the safety of energetic materials before their testing; MARK HOFFMAN, a formulations chemist responsible for formulating high explosives for unique applications within strict safety, performance, and compatibility guidelines; LAWRENCE FRIED, a theoretical chemist who screens candidate high-explosives molecules using advanced computer codes; and PHILIP PAGORIA, an organic chemist, who is expert in synthesizing new high-energetic compounds.

On the Offensive against Brain Attack

Under the leadership of the Laboratory's Center for Healthcare Technologies, a multidisciplinary team is developing a variety of much-needed tools to provide stroke victims with early, aggressive diagnosis and treatment.

IN the fall of 1994, a group in Lawrence Livermore National Laboratory's Center for Healthcare Technologies began asking a pointed question whose answer was to profoundly affect the focus of a major part of the Center's research: Given that both heart attack and stroke result from disruption of blood flow, why are cardiovascular conditions treated with aggressive medical intervention while cerebrovascular conditions usually receive passive intervention with emphasis on rehabilitation? Why is stroke not treated as "brain attack"? The answer, they found, was not that there is something fundamentally different about the two potentially deadly maladies. Instead, what they found was that doctors frequently did not have the proper tools to treat stroke as quickly and aggressively as they treat heart attack.

Heart attacks and strokes usually result from decreased blood flow interrupting the supply of oxygen and nutrients to tissue. Most frequently, the flow is decreased because of a blockage, but flow can also be disrupted by malformations or rupture of the vessels. An important difference between a heart attack and a stroke is that the size of the blood vessels involved in a stroke are significantly smaller. Recognizing that Lawrence Livermore has capabilities in microfabrication and other technologies that could be used to reduce the size of medical devices, the Center for Healthcare Technologies established a program to create a new standard of stroke care.

Critical to defining this standard was the "Workshop on New Technology for the Treatment of Stroke," which the Center sponsored in March 1995. The workshop was attended by internationally recognized stroke clinicians and researchers, cardiologists with experience in medical devices used to treat heart attack, and scientists and engineers from Lawrence Livermore and Los Alamos national laboratories. Instead of the typical conference agenda of success stories, clinicians described significant areas of unmet need for diagnosing and treating stroke victims, particularly the want of medical devices that might satisfy those needs.

Out of the workshop grew a vision of the future of stroke care and a framework for the priorities of a multidisciplinary team of Laboratory researchers who, with the help of Laboratory Directed Research and Development funding, are developing much-needed tools to diagnose and treat stroke. The Lawrence Livermore stroke initiative team's vision of the future of stroke care is summarized in Figure 1. It focuses on the greatest unmet clinical needs—restoring blood flow, preventing hemorrhage, improving treatment decisions with sensors, and identifying the at-risk population with new screening technologies. (For a primer on the kinds, causes, and treatment of stroke, see the box on p. 19.)

The Livermore team consists of specialists in biomedical engineering, biology and bioscience, laser medicine and surgery, micro-engineering, microsensors, and computer simulation. It also has key collaborators from academic medical centers and private companies. These partnerships are the basis for rapidly moving the medical device concepts from the research laboratory through development, clinical trials, regulatory approval, and manufacture so that the resulting new tools can have a timely impact on the lives of the thousands of people who have strokes each year.

Since the workshop, the stroke-initiative team's research has developed several proof-of-principle prototypes. The work falls into four categories: microsensors for brain and clot characterization, optical therapies for breaking up clots in the blood vessels of the brain, laser–tissue interaction modeling, and microtools for treating aneurysms (a leading cause of hemorrhagic stroke).

Sensors to Diagnose Clots

The Laboratory's stroke initiative has made substantial progress in developing microsensors that improve understanding of the biochemistry of stroke as well as offer the potential to improve stroke diagnosis, monitoring, and treatment. The sensors have the potential to identify the types of clots that cause stroke, to monitor patients during therapies that dissolve clots or protect brain cells with drugs, and to determine the health of brain or blood vessel tissue at a stroke site prior to treatment.

Development and use of these sensors, like much of the team's work, are predicated on the availability of microcatheters. These tiny, hollow tubes, which are available from a number of manufacturers, can contain optical fibers to which microsensors and other diagnostic, treatment, and monitoring tools being developed at the Laboratory are attached (Figure 2). Inserted in the femoral artery, the microcatheters are guided by microwires through the circulatory system to the clot

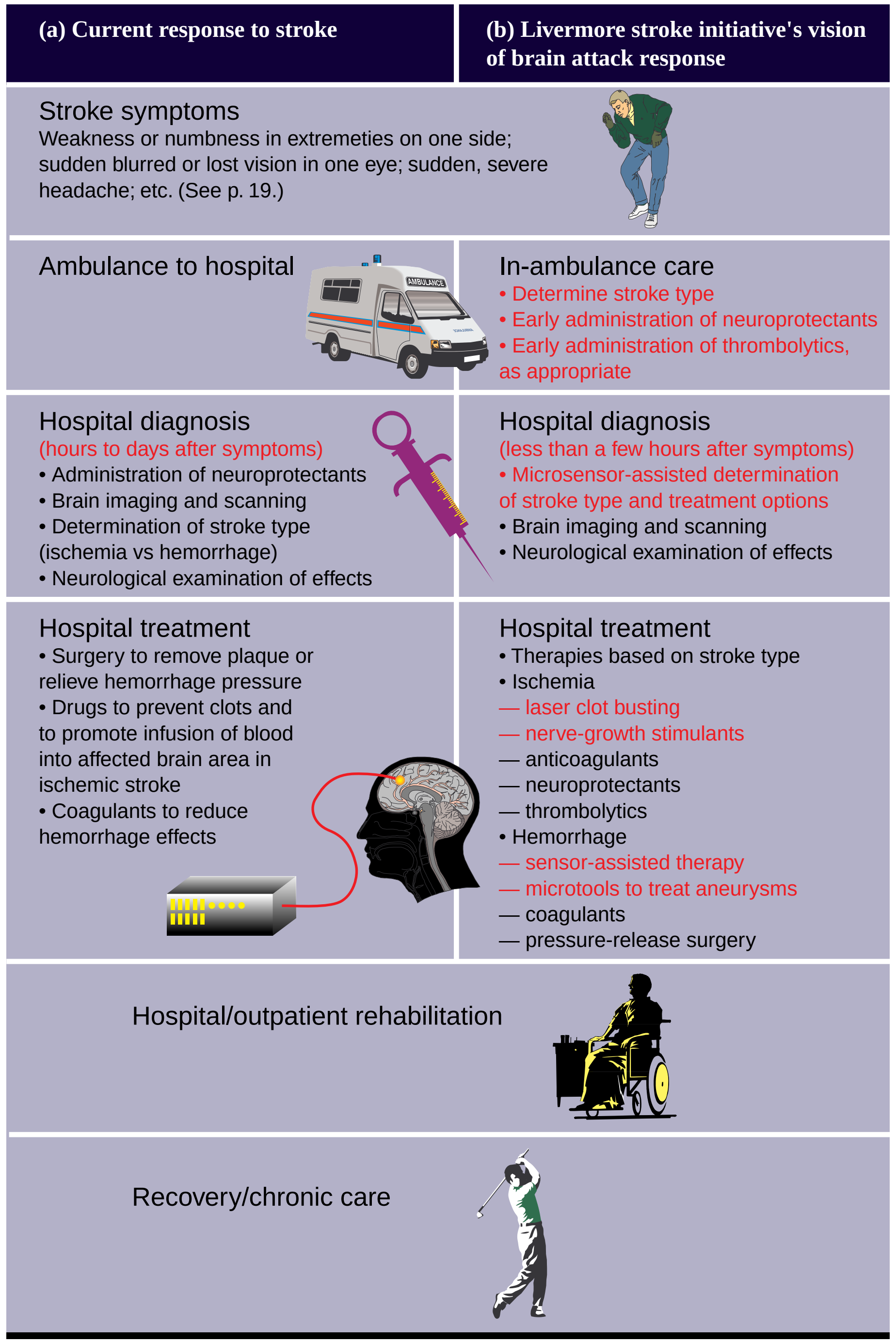


Figure 1. (a) Current response to stroke is more passive than active and lacks urgency largely because of the want of tools to diagnose and treat stroke early. The more time that passes after a stroke, the less the chance of even partial recovery from its effects. (b) The overriding goal of the Laboratory's stroke initiative is to improve those chances through early intervention. The Center for Healthcare Technologies' vision for the future of stroke care concentrates on providing tools for early, aggressive medical intervention to improve a stroke victim's chances for full recovery or more productive rehabilitation.

site in the brain where the tools attached to them can do their work to combat brain attack.

Lawrence Livermore researchers have, for example, demonstrated *in vitro* fiber-optic and electrochemical sensors for measuring pH at stroke sites.[1] These sensors can establish brain tissue viability by direct measurement of pH in brain tissue or through indirect measurement in blood near the stroke site. Livermore scientists have developed miniature intracranial (direct brain tissue) electrochemical and fiber-optic pH sensors, which neurosurgeon collaborators at the State University of New York at Buffalo have used for *in vivo* animal testing.

The measurement of blood pH is one of a number of chemical "markers" that have been identified to assess the health of blood-vessel tissue at the site of a stroke, thereby providing guidance in stroke therapy. When tissue dies, lactic acid builds up and blood pH decreases. So if blood pH is below normal (7.4) at or near the stroke site, then brain cell death has occurred, and the use of neuroprotectant drugs to minimize brain damage is unwarranted. If, on the other hand, pH is close to normal, cell death has not occurred, and neuroprotectant drugs become a therapeutic option.

In the Laboratory's fiber-optic pH sensor, a pH-sensitive dye, seminaphthorhodamine-1 carboxylate (SNARF-1C), is mixed with transparent silica sol-gel and dip-coated onto an optical fiber tip. In laboratory tests, the tip is placed in blood, and the dye is excited by a tungsten–halogen light source or a low energy density laser. The emission spectra of the dye is pH sensitive. These tests showed that the sensor had good sensitivity in the pH range of 6.8 to 8.0, indicating possible use for *in vivo* sensing of blood pH in the neighborhood of a stroke site.

Livermore scientists are also developing a D-dimer biosensor to monitor stroke patients during therapies

to dissolve blood clots in the vessels of the brain. D dimer is a substance with antigenic properties (i.e., capable of stimulating an immune response) and is produced as a result of a complex biochemical process when clot-dissolving drugs are injected via a microcatheter into blood clots.

Livermore's D-dimer biosensor can act as a diagnostic tool by indicating whether the blockage is caused by plaque or by a clot. Clot-dissolving drugs will not dissolve plaque; therefore, if an elevated concentration of D dimer is not detected at the site of blockage, then the blockage may be caused by something other than a clot, and alternative therapy is needed. In addition, because treatment using clot-dissolving drugs is highly variable, the D-dimer biosensor could help eliminate the guesswork related to the dosage and infusion rates. It could help physicians develop a diagnosis and treatment plan faster and reduce the risk of hemorrhage resulting from treatment to dissolve clots.

Medical Photonics

Members of the stroke-initiative team are developing a catheter-based system that uses laser energy to break up clots. The system will deliver low-energy laser pulses through a fiber-optic microcatheter (Figure 3). The laser energy will be directed at a cerebral clot, and by conversion of optical light to acoustic stress waves, it will break up the clot and restore blood flow in cerebral arteries. The concept is simple. The challenge is to determine the proper pulse strength needed to break up the clot without harming viable vessel tissue.

Research has focused on the optical and mechanical material strength and failure properties of the clots and tissue found in the cerebral blood vessels.[2] Using a tunable optic parametric oscillator (OPO) laser system at Livermore's Medical Photonics Laboratory (Figure 4), the medical-lasers team has conducted *in vitro* experiments to send laser pulses

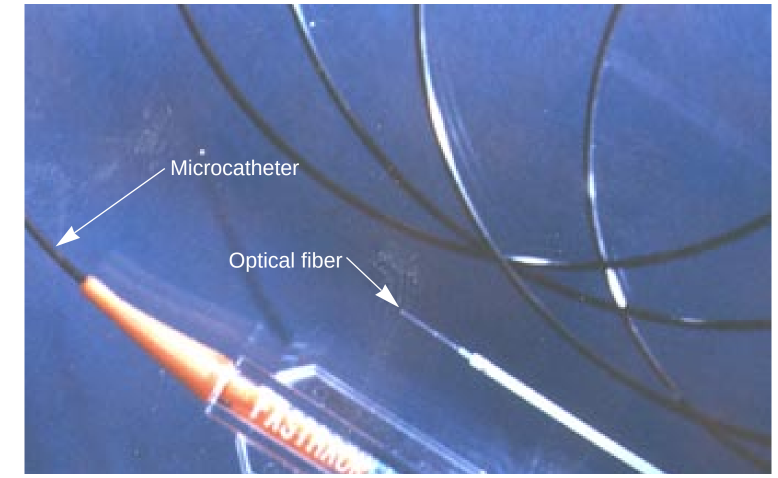


Figure 2. Optical fibers about the diameter of human hair can be enclosed in a hollow microcatheter and steered by microwires through the circulatory system to stroke sites in the brain. Microsensors and microtools are attached to these fibers to provide rapid, improved stroke diagnosis and treatment.

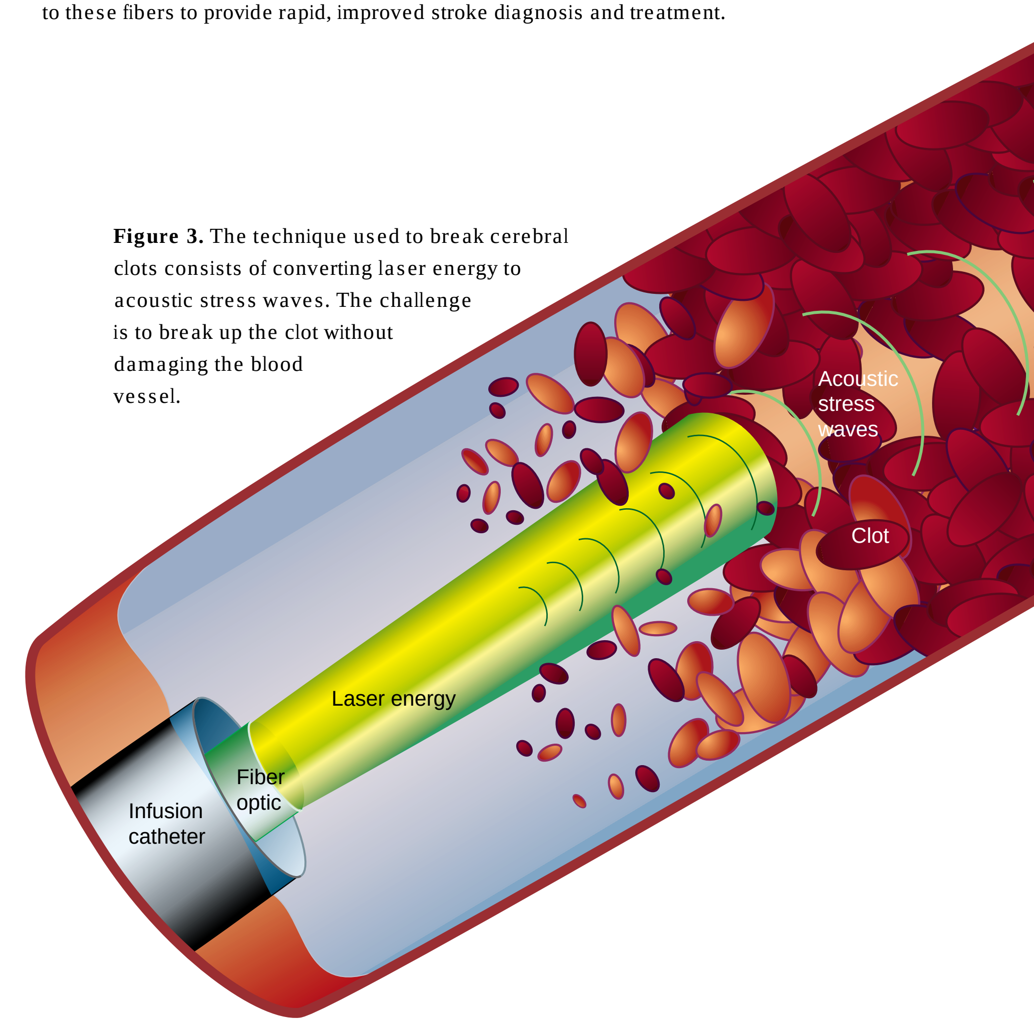


Figure 3. The technique used to break cerebral clots consists of converting laser energy to acoustic stress waves. The challenge is to break up the clot without damaging the blood vessel.

into a blood phantom (water colored with red food coloring). They have identified two distinct regimes of dynamic response, one due to strong laser light absorption, the other to moderate absorption.

In both cases, the confined stresses imparted to the liquid are substantial and determine most of the important dynamics. In the strong absorption case, energy is deposited in a thin zone near the fiber tip (Figure 5a). A thermally generated vapor bubble develops around the tip, and the initial stress wave, which can generate high peak pressure within 400 nanoseconds (billionths of a second), quickly propagates away from the tip. In the moderate case, energy is deposited in an extended zone beyond the fiber tip (Figure 5b). The initial stress evolves from the heated region within 500 micrometers (millionths of a meter) of the end of the tip, and the largest stress gradients, which develop within 20 nanoseconds, are directed radially and are situated in the immediate vicinity of the tip. Eventually (within 100 nanoseconds), a cloud of tiny bubbles develops in response to the stress caused by laser heating. In both cases, this expansion and collapse of bubbles exert pressure and shear forces on a clot, which lead ultimately to its breakup.

The Laboratory recently entered into a Cooperative Research and Development Agreement (CRADA) with EndoVasix Inc. of Belmont, California, which will eventually market the laser "clot-busting"

Figure 4. Livermore scientists use a tunable optic parametric oscillator (OPO) laser to create a series of laser back-lighted images (see Figure 5 below) of the pressure distribution of laser energy within a blood-like fluid.

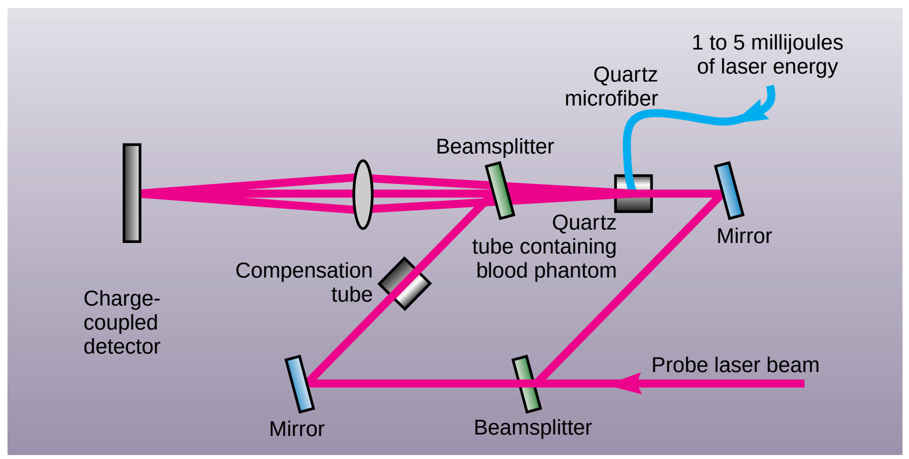
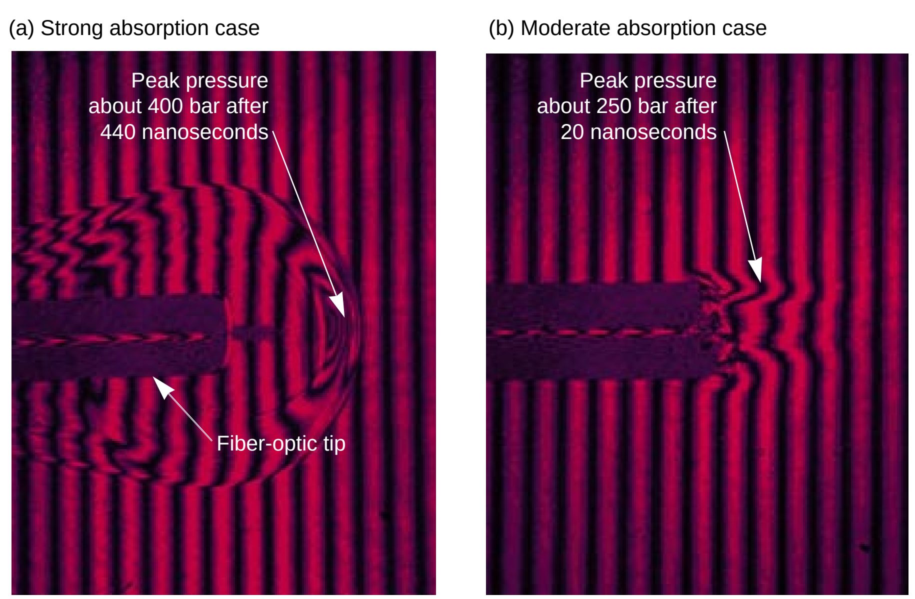


Figure 5. In laboratory experiments to develop a laser system to break up clots, Livermore researchers have identified two regimes of dynamic response. (a) In the strong absorption case, heat from the laser energy generates a vapor bubble about the fiber tip. (b) In the moderate case, initial stress evolves from the heated region very near the fiber tip. Within 100 nanoseconds, a cloud of tiny bubbles develops in response to the stress caused by laser heating. The expansion and collapse of these bubbles exert pressure and shear forces on the clot, ultimately leading to its breakup.



Brain Attack Facts*

Stroke (or "brain attack") results from vascular disease affecting the arteries supplying blood to the brain and occurs when one of these vessels bursts or is clogged. Part of the brain is deprived of the oxygen and nutrients it needs to function, the nerve cells die within minutes, and the part of the body controlled by these cells cannot function. Sometimes the devastating effects of stroke are permanent because the dead brain cells are not replaced.

Stroke is the leading cause of permanent disability in the U.S. and the third leading cause of death. Each year, 550,000 Americans have strokes. One-third of them die. Many of the survivors, who currently total over 3 million, have decreased vocational function (71%); of these 16% remain institutionalized, and 31% need assisted care. The personal cost is incalculable; the annual cost for treatment, post-stroke care, rehabilitation, and lost income to victims (but not their family caregivers) is $30 billion.

Types of Stroke

There are two main types of strokes, ischemic and hemorrhagic. Clots—cerebral thrombuses or cerebral embolisms—cause ischemic strokes. Cerebral hemorrhage or subarachnoid hemorrhage causes hemorrhagic strokes. Ischemic strokes are the most common, hemorrhagic strokes the most deadly.

Cerebral thrombosis occurs when a blood clot (a thrombus) forms in an artery in or leading to the brain, blocking the blood flow. It is the most common cause of ischemic stroke. Cerebral embolism occurs when a wandering clot (an embolus) or some other particle occurs in a blood vessel away from the brain, usually the heart. The clot is carried by the bloodstream until it lodges in an artery leading to or in the brain.

A cerebral hemorrhage occurs when an artery in the brain bursts, flooding the surrounding tissue with blood. Bleeding from an artery in the brain can be caused by a head injury or a burst aneurysm, a blood-filled pouch that balloons out from a weak spot in the artery wall. A subarachnoid hemorrhage occurs when a blood vessel on the surface of the brain ruptures and bleeds into the space between the brain and the skull (but not into the brain itself).

Hemorrhagic strokes cause loss of brain function both from loss of blood supply and from pressure of accumulated blood on surrounding brain tissue. The amount of bleeding determines the severity. If hemorrhagic stroke victims survive (which they do in 50% of the cases), their prognosis is better than that of ischemic stroke victims. With ischemic stroke, part of the brain dies and does not regenerate. With hemorrhagic stroke, pressure from the blood compresses part of the brain, but the pressure diminishes gradually and the brain may return to its former state.

About 10% of all strokes are preceded by "little strokes" called transient ischemic attacks (TIAs). They are more useful for predicting *if*, rather than *when*, a stroke will happen. They occur when a blood clot temporarily clogs an artery and part of the brain does not get the blood it needs. The symptoms, which are the same as stroke symptoms, occur rapidly and last a relatively short time, usually between 1 and 5 minutes. TIAs can last up to, but not more than, 24 hours. Unlike stroke, when a TIA is over, people return to normal, because the nerve cells were not deprived of oxygen long enough to die.

Diagnosis and Treatment

Diagnosing that a stroke has occurred and its type and severity takes time—time that stroke victims may not have. Diagnostic tools are tests that image the brain, such as computerized axial tomographic (CAT) scans, magnetic resonance imaging (MRI) scanning, and radionuclide angiography or nuclear brain scan. Tests that show the electrical activity of the brain are also used. The two basic tests of this type, an electro-encephalogram (EEG) and the evoked response test, measure how the brain handles different sensory stimuli such as flashes of light, bursts of sound, or electrical stimulation of nerves in an arm or leg.

Tests that show blood flow to and in the brain are also used for diagnosis. One of these is the Doppler ultrasound test, which can detect blockages in the carotid artery. Another is carotid phono-angiography, wherein a stethoscope or sensitive microphone is put on the neck over the carotid artery to detect abnormal sounds (bruits) that may indicate a partially blocked artery. Yet another is digital subtraction angiography, in which dye is injected into a vein in the arm and an x-ray machine quickly takes a series of pictures of the head and neck. From these x rays, doctors can determine the location of any blockages, how severe they are, and what can be done about them.

Surgery to remove plaque from artery walls, drugs that prevent clots from forming or getting bigger, acute hospital care, and rehabilitation are all accepted ways to treat stroke. Sometimes treating a stroke means treating the heart, because various forms of heart disease can contribute to the risk of stroke, particularly those caused by clots that form in a damaged heart and travel to the brain. But compared to the diagnosis and treatment tools that have been developed for heart attack, those for brain attack seem extremely limited and have not advanced greatly in recent years.

* *Heart and Stroke Facts* (The American Heart Association, Dallas, Texas, 1994), pp. 21–27. This booklet is available from the American Heart Association's National Center, 7272 Greenville Avenue, Dallas, Texas 75231-4596 (telephone: 1-800-242-8721).

technology. EndoVasix is investing in the development of a prototype system for clinical demonstrations beginning with animal stroke models. Some of the preliminary animal tests have already taken place.

Laser–Tissue Interaction

Central to the design of clot-busting tools is the refinement and use of computer codes for modeling laser–tissue interaction. Based on the laser–matter interaction codes developed for inertial confinement fusion at Livermore, the Laboratory's LATIS (laser–tissue) code provides a basis for predicting how short-pulse, low-energy medical lasers affect tissue.[3] It thus promote the rational design of clot-busting devices by modeling laser–tissue interaction during the process. By taking into account a raft of variables—size and composition of the clot, strength of blood-vessel tissue, and buildup and transport of heat during laser clot busting—this code can numerically simulate the hydrodynamics of the laser-created energy needed to break up clots and predict the amount of energy needed to do so without damaging other tissue.

The modeling team has made significant progress in simulating the laser clot-busting process with a focus on short-pulse (1- to 10-nanosecond) interactions of laser light with water and blood clots.[4] These advances in LATIS are being used to improve the laser clot-busting technology discussed earlier. They will be refined and expanded to better determine the parameters of the hydrodynamics at the heart of a safe, effective laser clot-busting system.

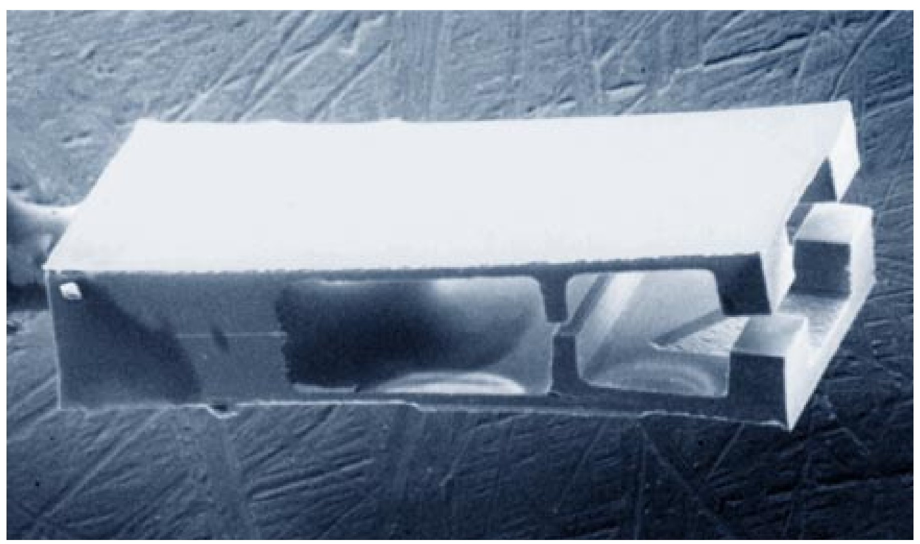


Figure 6. Microtools such as this silicon microgripper with "shape memory" will be used to treat the cerebral aneurysms that lead to hemorrhagic stroke. The microgripper is less than 1 cubic millimeter, that is, about the size of the head of a straight pin. (Approximate size: ▫)

The medical applications have also had positive "spin-back" to the core programs at the Laboratory. For instance, because the medical applications required simulation of how laser beams interact with highly scattering materials, a bug in one of the Monte Carlo x-ray transport subroutines used in national security applications was discovered and corrected.

Microtools

Miniaturization expertise from Lawrence Livermore's Microtechnology Center, Precision Engineering Group, and Plastic Shop has produced a variety of silicon, metal, and plastic microsensors and actuators for the stroke initiative. One of these with the potential to prevent strokes caused by hemorrhage rather than clots or other blockages is the "shape memory" microgripper (Figure 6). These tiny devices (less than a cubic millimeter) have a variety of applications, but the initial one is for treating aneurysms. Very fine metal thread is placed into the microgripper, which is connected to a guidewire cable and maneuvered to the site of the aneurysm. Closed, it slips into the aneurysm through the narrow neck connecting the aneurysm with the vessel wall. Once inside, the microgripper's heater is activated by power sent through the guidewire tether, and the gripper opens, releasing the metal thread into the aneurysm. The gripper then cools, "remembers" its closed shape, and can be withdrawn through the neck, leaving behind the metal thread. The thread embolizes (acts as a clot in) the aneurysm, reducing blood flow and pressure in the aneurysm. Without the pressure, the aneurysm eventually fills with scar tissue and is significantly less likely to rupture and cause a hemorrhagic stroke.

New Vision of Stroke Cure

The work of the stroke initiative at Lawrence Livermore hopes to remedy the paucity of tools for diagnosing and treating strokes. Its vision of stroke care includes medical devices for screening people without symptoms for stroke risk. It places special emphasis on the development of tools to provide earlier rather than later diagnosis of stroke type and assessment of brain cell damage so that appropriate treatment can be initiated rapidly. It has guided Livermore researchers in the development of technology to break up stroke-causing clots with laser energy as well as microsensors and microtools to assist in the diagnosis and treatment of various kinds of brain attack. And it looks forward to providing the means for more instances of full recovery, fewer stroke-related disabilities, and less need for chronic care.

—Dean Wheatcraft

Key Words: brain attack, laser "clot-busting," laser–tissue interaction modeling, LATIS code, medical photonics, microsensors, neuroprotectant drugs, shape-memory microgripper, stroke.

References

1. Sheila A. Grant and Robert S. Glass, *Sol-Gel-Based Fiber-Optic Sensor for Blood pH Measurement*, Lawrence Livermore National Laboratory, Livermore, California, UCRL-JC-125297 (January 1997). (Submitted to *Analytica Chemica Acta*.)
2. P. Celliers et al., "Dynamics of Laser-Induced Transients Produced by Nanosecond Duration Pulses" *Proceedings of the Society of Photo-Optical Instrumentation Engineers*, **2671A** (1996).
3. R. A. London et al., *Laser–Tissue Interaction Modeling with LATIS*, Lawrence Livermore National Laboratory, Livermore, California, UCRL-JC-125974 (February 1997). (To be published in *Applied Optics*.)
4. M. Strauss et al., "Computational Modeling of Laser Thrombolysis for Stroke Treatment," *Proceedings of the Society of Photo-Optical Instrumentation Engineers*, **2671** (1996).

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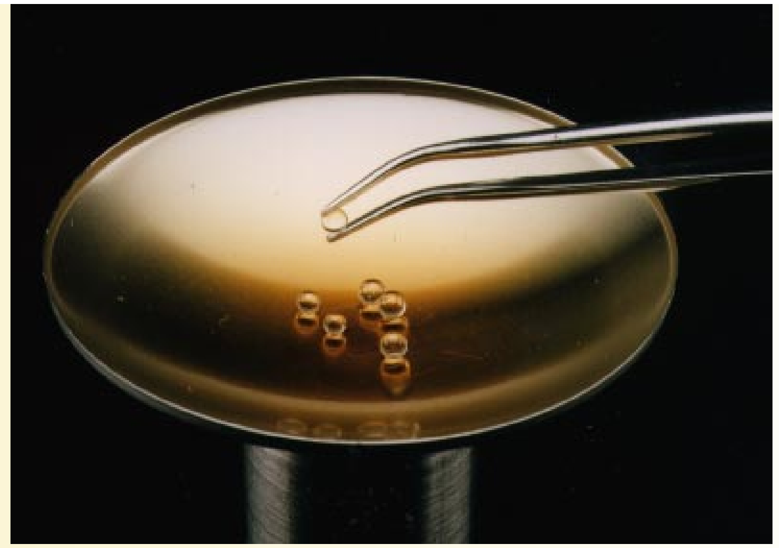
About the Team

The stroke-initiative team at the Laboratory is a multidisciplinary group of scientists and engineers from several directorates—Biology and Biotechnology, Engineering, Laser Programs, Physics and Space Technology, Defense and Nuclear Technologies, and Chemistry and Materials Science. The team's members have combined their expertise in biomedical engineering, biology and bioscience, laser medicine and surgery, micro-engineering, microsensors, and computer simulation to create a variety of tools to respond quickly and urgently to brain attack and thereby improve the chances of a stroke victim's survival and recovery. They are collaborating with academic medical centers and private companies to move these proof-of-principle prototypes as quickly as possible from the research stage to development, clinical trials, regulatory approval, and manufacture so that they can benefit as soon as possible the lives of people who have strokes. Pictured left to right are: ABRAHAM LEE, ROBERT GLASS, WILLIAM BENETT, LUIZ DA SILVA, PATRICK FITCH, RICHARD LONDON, SHEILA GRANT, and STEVEN VISURI. (Not shown are PETER CELLIERS, PETER KRULEVITCH, and DENNIS MATTHEWS.)

Laser Targets
The Next Phase



Two-millimeter, poly(alpha-methylstyrene) (PAMS) bead mandrels are rolled in a small, tilted, slowly rotating pan until evenly coated with plasma polymer. Heat treatment decomposes the PAMS and it diffuses through the plasma polymer coating, leaving behind smooth, spherical, thin-walled hollow shells that are the targets for laser fusion experiments.

IT will take a community of workers to bring the goals of the National Ignition Facility (NIF) to fruition. While national attention has been focused on the funding and construction of the 192-beam laser facility, scientists at Lawrence Livermore are working on myriad problems whose solutions are necessary to NIF's success. A group of materials scientists, for example, is developing techniques to produce round, hollow shells about 2 millimeters in diameter—smaller than BB-gun pellets. This work seems incongruous in a project dominated by a football-stadium-size facility. But when filled with deuterium or deuterium–tritium fuel, these shells become the targets for NIF's inertial confinement fusion (ICF) experiments. The goal of these experiments is to create fusion ignition—intense temperatures and pressures like those at the centers of stars for a small fraction of a second.

Steve Letts and Evelyn Fearon of the Laser Programs Directorate's Target Area Technology Program are among the materials scientists continuing Lawrence Livermore's more than 20 years of research and development on laser targets. Their focus now is on targets for NIF experiments. With 40 times more energy and 10 times more power than Nova (currently the world's largest operating laser), NIF will require targets about 2 millimeters in diameter, 4 times larger than those used previously, which are about half a millimeter in diameter.

The increased shell size must be achieved in tandem with making the shell very smooth and symmetrical. During an ICF experiment, extremely high laser energies are absorbed by the fuel capsule, causing the capsule wall to blow off with such tremendous force that the fuel inside is compressed to very high density. This compression, which must be as uniform as possible, is necessary for ignition. Any capsule surface or shape irregularities constitute perturbations that will grow in amplitude during implosion, because of hydrodynamic (Rayleigh–Taylor) instabilities (see *Energy & Technology Review*, April 1995, pp. 1–9). The perturbations cause the inner wall of the capsule to mix with the fuel, cooling it and thereby degrading efficiency.

The Progression of ICF Targets

Letts and Fearon's technique for making shells uses an entirely new approach. Previously, plastic shells were produced when droplets of polystyrene solution were dropped down a heated drop tower, where evaporation first caused a skin to form on the droplets and then further vaporization of the solvent inside the skin caused the droplets to expand into hollow shells.

Because the drop-tower technique produced shells of a limited size range, researchers tried micro-encapsulation techniques to increase shell sizes. They encapsulated droplets of water in a polymer solution suspended in an aqueous phase; the solvent containing the polymer would slowly dissipate into the aqueous phase, leaving behind a polymer shell. However, the resulting shells were uneven in thickness and had bubbles in their walls. Steve Letts explains that these techniques frequently "wouldn't produce round shells most of the time, so those that were round would have to be carefully picked out—not an easy task with such tiny things."

He came up with a new idea. While measuring mass loss in polymers when they were heated, he identified one polymer material that evolved into a gas when heated to about 300°C, disappearing cleanly without any trace or residue. He figured out a way to take advantage of the material's unique combination of characteristics.

That material was poly(alpha-methylstyrene), or PAMS. In Letts's new fabrication method, an amount of PAMS is shaped into a smooth sphere, or mandrel, which is overcoated with a thermally stable plasma polymer to a desired thickness. The overcoated mandrel is heated to about 300°C, at which temperature the PAMS depolymerizes (decomposes) into a gas, diffuses through the plasma polymer overcoat (which is thermally stable up to 400°C), and leaves behind a hollow plasma polymer shell (see the figure on p. 23).

Letts postulated that this method would be feasible for producing fuel capsules of the size needed for NIF if a suitable PAMS mandrel could be formed. In addition, because the shell is built outward from the PAMS mandrel, it might be feasible to incorporate various layers during the overcoating process, which would be useful for diagnosing shell performance. The method would be successful if good quality mandrels could be made, an even overcoat could be deposited on the mandrel, and pyrolysis (heat treatment) could be accomplished without distorting or collapsing the resulting shell.

Spherical, Smooth Mandrels

Evelyn Fearon coordinated PAMS mandrel production. She and the other fabricators ground commercial PAMS beads into smaller sizes, put them through a sieve, and suspended them in a water solution hot enough to soften them, thus taking advantage of surface tension to pull the bead into a sphere. Bead surfaces were smoothed further by exposing them to solvent vapor while dropping them down a heated column. During the drop, the bead's thin surface layer dissolved and dried, leaving a surface roughness of less than a billionth of a meter (as measured by an atomic-force microscope).

Smooth, spherical bead mandrels were fairly easy to make. However, they tended to distort from the heat generated during overcoating and become nonsymmetrical or coat unevenly. To overcome the heat effects, Fearon experimented with higher molecular weight PAMS and lowered the overcoating temperature, but the adjustments did not wholly overcome the distortion problem.

The Target Area group turned to hollow mandrels made by micro-encapsulation and supplied by General Atomics of San Diego, California, another DOE contractor. Hollow mandrels have two advantages. They contain less PAMS to depolymerize, and thus, less force is exerted on the overcoat during depolymerization. Second, higher molecular weight PAMS (96,000 versus 11,000 for beads) can be used to make them, because, unlike the beads, they do not need hot-water softening, which requires the lower molecular weight material. Because they are ultimately depolymerized, some wall unevenness and internal bubbles are tolerable, as long as the shells are spherical and their outer surface finishes are smooth. Compared with bead mandrels, the hollow mandrels have shown far less distortion during overcoating and pyrolysis.

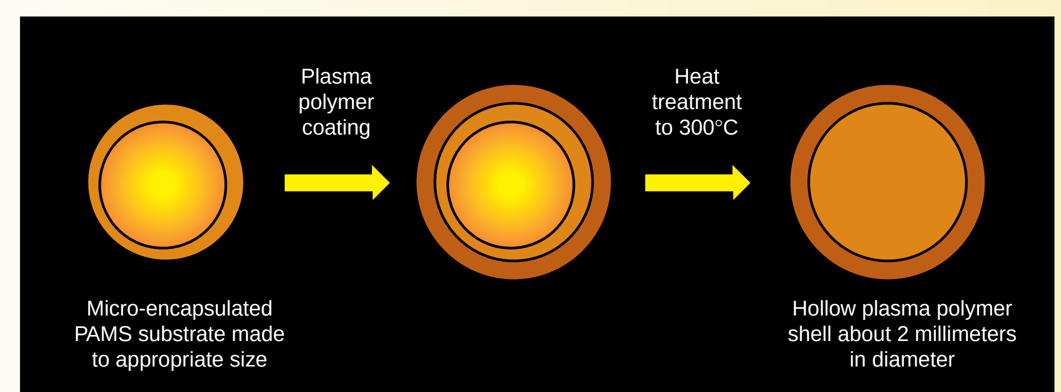
An Even Coat of Plasma Polymer

Plasma polymer is well suited to be fuel–shell material. It is transparent, which allows fusion experimenters to diagnose the contained fuel layer. It can be used to coat the mandrels because it can withstand PAMS pyrolysis temperatures and is permeable to the gaseous, depolymerizing PAMS.

In the coating technique used by the Target Area group, the mandrels are agitated in a bouncing pan in the plasma coating chamber or, in a variation, rolled in a tilted, slowly rotating pan until they are evenly coated (see the figure on p. 22). The crucial variables determining even coating are just the right amount of agitation and the correct (not-too-high) temperature.

Successful Pyrolysis

During pyrolysis, the shells can collapse, burst, deform, or shrink. While collapse is mainly caused by nonuniform coating, the other problems result from thermal effects. To avoid them, the researchers devised a temperature program that controls the rate of PAMS decomposition. It consists of raising the pyrolysis temperature by 10°C every minute until 200°C is reached, holding it there for 30 minutes to allow low-



Livermore scientists have developed a technique for producing hollow laser-target shells by starting with a hollow poly(alpha-methylstyrene) (PAMS) mandrel and then overcoating it with thermally more stable plasma polymer. The coated mandrel is heated to 300°C over 30 hours or more; the PAMS decomposes and passes through coating, leaving a spherical, hollow plasma polymer target shell.

temperature volatiles to escape, and then ramping it up by 0.2°C every minute up to 300°C, where it is held for 30 hours or more, depending on the size of the shell. The plasma polymer shrinks gradually and uniformly during pyrolysis, and thus sphericity is maintained. Experimenters observe and measure the shrinkage only to predict the size of a completed shell.

An optical microscope is used to measure the wall thickness and diameter of pyrolyzed shells, a scanning electron microscope is used to determine how smooth and free of particle defects shell surfaces are, and an atomic-force microscope is used to make detailed measurements of the sphericity and roughness of the shell.

Challenges Ahead

The techniques described here have now been adopted by General Atomics as the preferred method for making 0.5-millimeter-diameter capsule targets for Nova ICF experiments at Livermore and 0.9-millimeter-diameter capsules for ICF experiments at the Omega Laser facility at the University of Rochester. The success in moving this research proof of principle to actual target production is certainly encouraging. However, significant challenges still face Livermore's laser-target scientists.

Currently the development efforts at Lawrence Livermore are focused on adapting the technology developed by Letts and Fearon to the production of 2-millimeter-diameter capsules for NIF. This effort has two parts. The first, being led by Ken Hamilton, is to develop micro-encapsulation techniques to form PAMS microshells with the required outer surface sphericity and surface finish. To meet NIF specifications, these shells must be no more than 1 micrometer, or a millionth of a meter, out of round; that is, the radius to the outer surface can vary by no more than 1 micrometer (out of 1,000) as one moves across the surface. Solving this extremely difficult problem will require significant improvements in current micro-encapsulation technology. Once it is solved, the second part will be to maintain the sphericity of the shell through the coating and thermal treatment to remove the PAMS.

Members of the Laboratory's Target Area Technology Program will continue to refine laser target technology. Beyond making targets for current ICF experiments, they must focus on developing targets for the real NIF event—ignition. The PAMS technique is being investigated for that use.

—Gloria Wilt

Key Words: laser target, National Ignition Facility (NIF), inertial confinement fusion (ICF), fuel capsule, plasma polymer, polymer shell, micro-encapsulation, poly(alpha-methylstyrene) (PAMS), hydrodynamic instability.

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Patents and Awards

Each month in this space we report on the patents issued to and/or the awards received by Laboratory employees. Our goal is to showcase the distinguished scientific and technical achievements of our employees as well as to indicate the scale and scope of the work done at the Laboratory.

Patents

Patent issued to	Patent title, number, and date of issue	Summary of disclosure
John S. Toeppen	**Method for Optical and Mechanically Coupling Optical Fibers** U.S. Patent 5,560,760 October 1, 1996	An inexpensive technique to splice optical fibers that does not cause deformation of the host fibers, does not require repeated thermal cycling of the optical fibers, does not cause thermal and photonic degradation of the fibers even at high power applications, does not cause the fibers to prematurely deteriorate with age, and is suitable for use with optical fibers having a core diameter of as much as 1,000 micrometers or greater. A solder–glass frit having a melting point lower than the melting point of the optical fibers is used to splice the two optical fibers together.
Rex Booth	**Charge Line Quad Pulser** U.S. Patent 5,563,457 October 8, 1996	A quartet of parallel coupled planar triodes that is removably mounted in a quadrahedron-shaped PCB structure. Releasable brackets and flexible means attached to each triode socket make triode cathode and grid contact with respective conductive coatings on the PCB and with a detachable cylindrical conductive element enclosing and contacting the triode anodes.The configuration permits quick and easy replacement of faulty triodes. By such orientation, the quad pulser can convert a relatively low and broad pulse into a very high and narrow pulse. A maximum impedance mismatch within a quartet planar triode circuit of less than 10% is maintained.
Thomas E. McEwan	**Precision Digital Pulse Phase Generator** U.S. Patent 5,563,605 October 8, 1996	A timing generator comprising a crystal oscillator connected to provide an output reference pulse. A resistor–capacitor combination is connected to provide a variable-delay output pulse from an input connected to the crystal oscillator. A phase monitor is connected to provide duty-cycle representation of the reference and variable-delay output pulse phase. An operational amplifier drives a control voltage to the resistor–capacitor combination according to currents integrated from the phase monitor and injected into summing junctions. A digital-to-analog converter injects a control current into the summing junctions according to an input digital control code.
Kurt H. Weiner Thomas W. Sigmon	**Process for Forming Retrograde Profiles in Silicon** U.S. Patent 5,565,377 October 15, 1996	A process for the formation of retrograde profiles in silicon, either previously doped crystalline or polycrystalline silicon, or for introducing dopant into amorphous silicon so as to produce the retrograde profiles. This process involves the formation of higher dopant concentrations in the bulk than at the surface of the silicon. By this process, n- and p-well regions in CMOS (complementary metal oxide silicon) transistors can be formed by a simple, flexible, and inexpensive manner. This technique has particular application in the manufacture of silicon integrated circuits where retrograde profiles are desired for the n- and p-well regions of CMOS transistor technology and for buried collectors in bipolar transistors.
Daniel W. Shimer Arnold C. Lange	**E-Beam High Voltage Switching Power Supply** U.S. Patent 5,566,060 October 15, 1996	A circuit device for generating a ground-level voltage feedback signal for controlling the output voltage of one of a plurality of dc–dc converter modules having their outputs connected in series to form a supply output lead. Each module includes a switching device for producing a pulsating voltage of controlled duty cycle, an inductor mechanism for converting the pulsating voltage into a smooth direct current, and an inverter mechanism for producing from the direct current an alternating current through the primary of a transformer. The transformer has at least one secondary winding inductively coupled to the primary winding for producing an output voltage of the module.

Patent issued to	Patent title, number, and date of issue	Summary of disclosure
George P. Roberson Michael F. Skeate	**Image Matrix Processor for Fast Multidimensional Computations** U.S. Patent 5,566,341 October 15, 1996	An apparatus for multidimensional computation that comprises a computation engine, including a plurality of processing modules. The processing modules are configured in parallel and compute respective contributions to a computed multidimensional image of respective two-dimensional data sets. A storage system is provided that stores the multidimensional data sets, and a switching circuit routes the data among the processing modules in the computation engine and the storage system. The processing modules include a programmable local host, by which they may be configured to execute a plurality of different types of multidimensional algorithms.
Gary W. Johnson	**Apparatus for Controlling the Scan Width of a Scanning Laser Beam** U.S. Patent 5,568,255 October 22, 1996	A system whereby the scan width of a swept ring-dye laser or a semiconductor diode laser can be measured and controlled in real-time with a resolution better than 0.1%. Scan linearity, or conformity to a nonlinear scan waveform, can be measured and controlled. The system consists of a Fabry–Perot interferometer, three CAMAC interface modules, and a microcomputer running a simple analysis and proportional-integral control algorithm. With additional modules, multiple lasers can be simultaneously controlled. Also included is an embodiment implemented on an ordinary personal computer with a multifunction plug-in board.
Kurt H. Weiner	**Method for Shallow Junction Formation** U.S. Patent 5,569,624 October 29, 1996	A doping sequence that reduces the cost and complexity of forming source/drain regions in complementary metal oxide silicon (CMOS) integrated circuit technologies. The process combines the use of patterned excimer laser annealing, dopant-saturated spin-on glass, silicide contact structures, and interference effects created by thin dielectric layers to produce source and drain junctions that are ultrashallow in depth but exhibit low sheet and contact resistance. The process uses no photolithography and can be achieved without the use of expensive vacuum equipment. The process margins are wide, and yield loss due to contact of the ultrashallow dopants is eliminated.
Alexander R. Mitchell Philip F. Pagoria Robert D. Schmidt	**Vicarious Nucleophilic Substitution to Prepare 1,3-Diamino-2,4,6-Trinitrobenzene or 1,3,5-Triamino-2,4,6-Trinitrobenzene** U.S. Patent 5,569,783 October 29, 1996	A process that is milder and more environmentally benign to easily convert nitroaromatic compounds to DATB, TATB, or mixtures thereof by using processes that avoid strong acids (H_2SO_4, HNO_3) at elevated temperatures (100 to 150°C) and the need for noxious materials such as ammonia, thionyl chloride, and hydrogen sulfide. DATB and TATB can be useful specialty explosives. TATB can also be used for the preparation of benzenehexamine, a starting material for the synthesis of novel materials such as optical imaging devices, liquid crystals, and ferromagnetic compounds.
Howard Nathel John H. Kinney Linda L. Otis	**Method for Detection of Dental Caries and Periodontal Disease Using Optical Imaging** U.S. Patent 5,570,182 October 29, 1996	A method of optical imaging that may be used both for the detection of dental caries and for the diagnosis and monitoring of gingivitis. Optical radiation is used in the wavelength region between 500 and 1,400 nanometers, where carious dental tissue is much more strongly absorbing than healthy tissue, so that transmitted or reflected optical radiation can be used to create a shadowgram of structures within the dental tissue. The same wavelength region used for the detection and location of tissue boundaries may be used to diagnose and monitor the progress and treatment of gingivitis.

Patent issued to	Patent title, number, and date of issue	Summary of disclosure
Joseph T. Salmon	**Split-Field Pupil Plane Determination Apparatus** U.S. Patent 5,570,189 October 29, 1996	An apparatus for locating a pupil plane following relay telescope optics along an optical path using a pair of optical wedges disposed side by side on the optical path for splitting an incident beam of collimated light on the optical path to provide two parallel side-by-side beams of collimated light on the optical path, the parallel side-by-side beams of collimated light being provided such that they diverge while being parallel to the path of the incident beam of collimated light.
George G. Pollock	**Precision Control of High Temperature Furnaces Using an Auxiliary Power Supply and Charged Particle Current Flow** U.S. Patent 5,597,501 January 28, 1997	A high-temperature furnace with two power supplies. A main power supply connected to a heating element in the furnace heats the furnace in the traditional manner. An auxiliary power supply introduces a current flow through charged particles between the heating element and an object holder. The main power supply provides the bulk heating power; the auxiliary provides temperature control.

Awards

Laboratory scientists **Paul Coronado**, **Dan Calef**, **Bob Sanner**, and **Lucy Hair** were recently selected by the **Society of Automotive Engineers** to be honored by the **Partnership for New Generation Vehicles** (PNGV) for their contribution to the development of affordable, energy-efficient, nonpolluting vehicles to get up to 80 miles per gallon. On March 31 in Washington, D.C., they received medals from Vice President Al Gore. PNGV is a collaboration of eight federal agencies, the U.S. Council for Automotive Research, Chrysler, Ford, General Motors, and 18 laboratories, among them Livermore, Los Alamos, and Sandia national laboratories. Its goal is to select the most promising new technologies by 1997 and produce a concept car by the year 2000. The Livermore team was honored for the development of aerogels to be catalysts for the next-generation vehicles. Sanner, a materials chemist, made materials that Coronado, a chemist, developed into aerogels, which were tested for use as a catalyst. Calef, a theoretical chemist, did modeling to determine which metals would or would not work in an aerogel environment, and Hair, a chemical engineer, served as principal investigator on the project.

Transforming Explosive Art into Science

Livermore researchers have studied and synthesized high explosives for decades because they are an integral element of every nuclear weapon. Today their work encompasses a wide range of basic research and programmatic activities. Researchers are combining breakthrough computer simulation codes, state-of-the-art experimental diagnostics, and a culture in which theoretical, synthesis, and experimental chemists and physicists work alongside each other. At the same time, they are working more closely with their partners in the energetic-materials community.

Lawrence Livermore chemists are synthesizing new compounds that yield more energy, are safer to store and handle, and are less expensive and more environmentally friendly to produce. They also are designing new paths to synthesizing existing energetic molecules that are cheaper and easier on the environment. In a parallel effort, experiments are being done to better understand the fundamental physics and chemistry of energetic materials, particularly with regard to their stability, sensitivity, and performance. Livermore chemists are also working to improve efficiencies in the production of these materials.

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On the Offensive against Brain Attack

The Center for Healthcare Technologies at Lawrence Livermore National Laboratory has undertaken a stroke initiative whose purpose is to provide the medical community with the tools that will allow doctors to diagnose and treat stroke as aggressively as they do heart attack. A multidisciplinary team of stroke-initiative researchers is collaborating with academic medical centers and private companies to move these tools from the research and development stage through clinical trials, regulatory approval, and manufacture so that they can benefit many thousands of people who have strokes each year. Tools the team has developed fall into four categories: microsensors for brain and clot characterization, a catheter-based system using laser energy to break up clots in the blood vessels of the brain, laser–tissue interaction models in support of laser "clot busting," and microtools for treating the aneurysms that cause hemorrhagic stroke.

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